Microactuators for biomorphic explorers: a few suggestions from theory

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A common problem facing the application of MEMS devices in many areas including biomorphic explorers is that the actuators proposed for use in these systems -- commmonly electrostatic actuators and bimetallic strips -- lack adequate work output and displacement magnitude. Substantial improvements in both these quantitities can be achieved by modifications of both material and design of actuators. On the material side, active materials show great promise because the underlying mechanism is a first order phase transformation. Further more, they allow designs where it is possible to combine the structural and actuator elements. In particular, shape-memory alloys are particularly attractive since they arguably have the largest work output per unit volume. Further, at small sizes the frequency of cycling is not limited because of fast heat transfer. However, the microstructure in films can be very different in thin films compared to the bulk and thus the shape-memory characteristics of a material can change. On the design side, we need to use configurations which allow us to use the full potential of the active behavior.

R.D. James and I have recently developed a theory of thin films which is suitable for martensitic materials and we have used it to study materials and designs for microactuators and micropumps[1]. This theory captures the change of microstructure as we go from bulk to thin films and moreover shows the need to use the films in "membrane" rather than "bending" mode for maximum work output. Based on this we have proposed materials systems and designs which are currently being experimentally evaluated by C.J. Palmstrom. Y.C. Shu and I have extended this theory to heterogeneous films -- polycrystalline and multilayer -- and have used it to study in particular the incluence of texture on the shape-memory effect. We show that sputtering texture is unfavorable for the shape-memory effect in common materials and propose other textures which yield large shape-memory effect.

The talk will report on these theoretical results, and on emerging efforts to find mechanisms for sub-millimiter aircraft[4]. The talk will also describe recent efforts in designing and constructing a shape-memory mini-crawler using lessons drawn from the above research.

1. K. Bhattacharya and R.D. James, A theory of thin films of martensitic materials with applications to microactuators, To appear in J. Mech. Phys. Solids, 1998.

2. Y.C. Shu and K. Bhattacharya, The influence of texture on the shape-memory effect in polycrystals, To appear in Acta Materialia, 1998.

3. Y.C. Shu, Heterogeneous thin films of martensitic materials, In preparation, 1998.

4. AFOSR MURI on "Computational Tools for the Atomistic/Continuum Interface: Nanometer to Millimeter Scale Aircraft". Website: http://www.multiscale.umn.edu

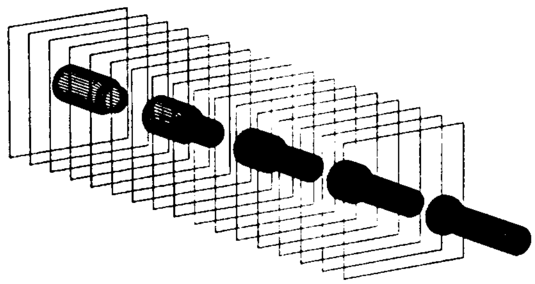
Microactuators of active materials

Kaushik Bhattacharya
Richard D. James
Yi-Chung Shu
Georg Dolzmann

Announcement

Interdisciplinary Research Program

Computational Tools for the Atomic/Continuum Interface: Nanometer to Millimeter Scale Aircraft



Prospective Graduate Students and Postdoctoral Fellows from engineering, physics and mathematics with outstanding records are encouraged to apply for a highly interdisciplinary basic research program on the forefront of science and engineering. The research concerns the development of new concepts for flight at nanometer to millimeter scale, with applications to atmospheric flight and to the design of vehicles for microsurgery. The general framework for this research is the propulsion of small vehicles by the motion of active materials - ferroelectric, magnetostrictive and shape memory materials - configured as deformable tubes, flaps or flagella and powered by a remotely applied electromagnetic field. The research is based in scientific computation, with additional opportunities in mathematical modeling and laboratory research. Specific research areas include:

1. Fluid mechanics and aerodynamics at nanometer to millimeter scale
2. Phase transformations and the behavior of active materials at small scales
3. Computational methods for the passage from atomic to continuum scales
4. The synthesis of active materials by molecular beam epitaxy
5. The design of micro-electro-mechanical (MEMS) systems for small scale flight

The participants with a brief summary of their fields are listed below. Interested persons are encouraged to contact any of the participants by e-mail for further information and application materials. For general information on the project, contact R. D. James, james@aem.umn.edu.

Kaushik Bhattacharya, *Applied Mechanics, California Institute of Technology,* Shape memory materials, active thin films, continuum mechanics of materials. bhatta@cco.caltech.edu

Iain D. Boyd, *Mechanical and Aerospace Engineering, Cornell University,* Computational fluid dynamics at the atomic continuum interface, Monte Carlo methods. boyd@mae.cornell.edu

Graham V. Candler, *Aerospace Engineering and Mechanics, University of Minnesota,* Computational fluid dynamics at the continuum/atomic interface aerodynamics. candler@aem.umn.edu

Richard D. James, *Aerospace Engineering and Mechanics, University of Minnesota,* Shape memory and magnetostrictive materials, active thin films, mathematical methods for change-of-scale. james@aem.umn.edu

Mitchell Luskin, *School of Mathematics, University of Minnesota,* Computational materials science, microstructure, phase transformations. luskin@math.umn.edu

Chris J. Palmstrøm, *Chemical Engineering and Materials Science, University of Minnesota,* MBE of thin films of microelectronic, magnetic and active materials. palms001@gold.tc.umn.edu

Karin M. Rabe, *Applied Physics and Physics, Yale University,* Density Functional Theory predictions of atomic level structural properties of active materials, effective Hamiltonians for ferroelectrics and related materials. rabe@critical.eng.yale.edu

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Facilities for the research include a dedicated multiprocessor machine for simulation, advanced molecular beam epitaxial system for the growth of thin films, clean room facilities for the analysis and patterning of thin films.

This research is supported by the Department of Defense Multidisciplinary Research Program (MURI), administered by the Air Force Office of Scientific Research

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Work per Unit Volume for Various Microactuators

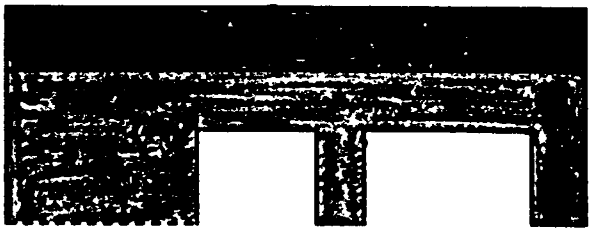
Krulevitch et al.

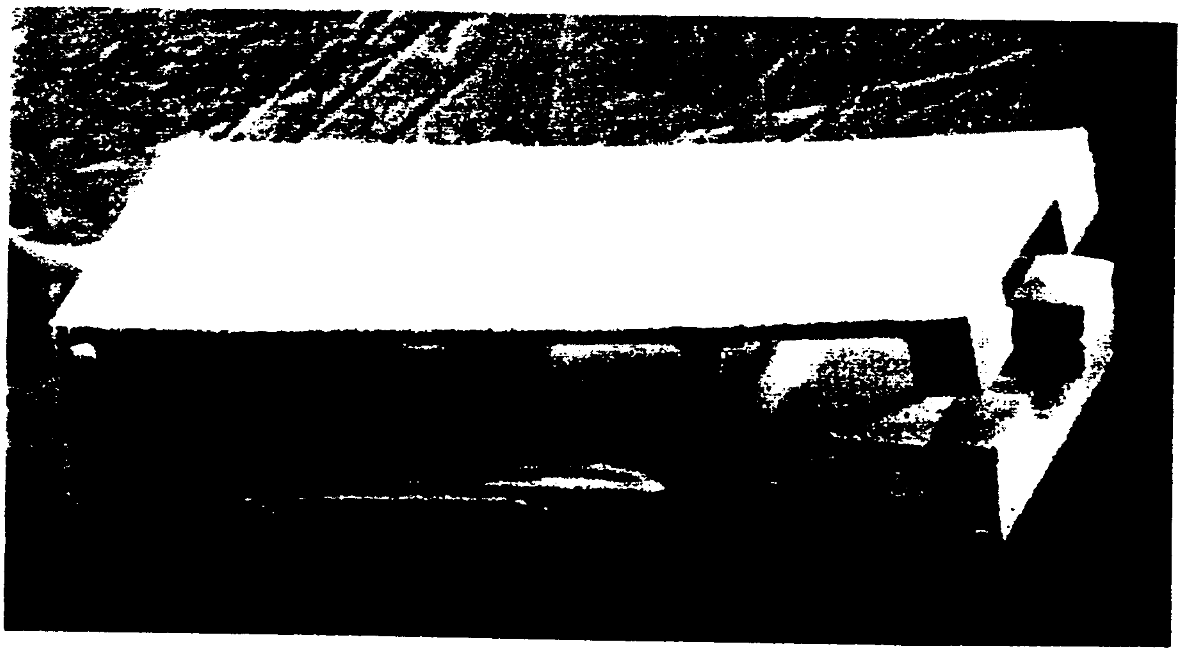
ACTUATOR TYPE	W/ v (J/m^3)
1. Ni - Ti SMA	2.5×10^7 6.0×10^6
2. Solid-Liquid Phase Change	4.7×10^6
3. Thermopneumatic	1.2×10^6
4. Thermal Expansion	4.6×10^5
5. Electromagnetic	4.0×10^5 2.8×10^4 1.6×10^3

ACTUATOR TYPE	W/ v (J/m^3)
6. Electrostatic	1.8×10^5 3.4×10^3 7.0×10^2
7. Piezoelectric	1.2×10^5 1.8×10^2
8. Muscle	1.8×10^4
9. Microbubble	3.4×10^2

Shape-memory Microgripper

Krulevitch et al.

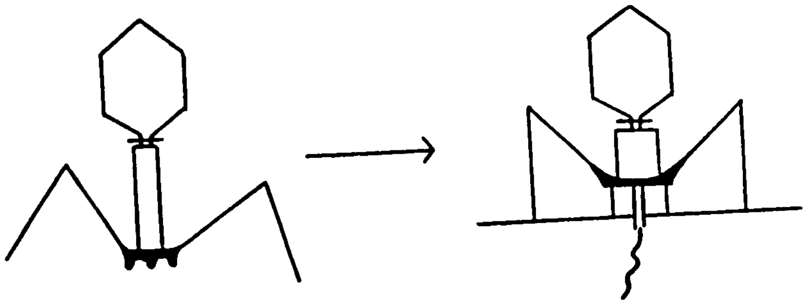


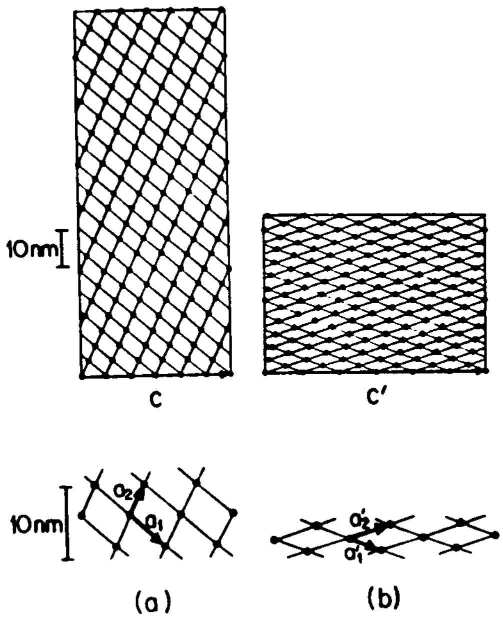


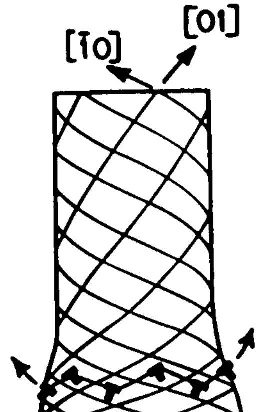
Size : 900 × 380 × 200 μm

T - 4 Bacteriophage

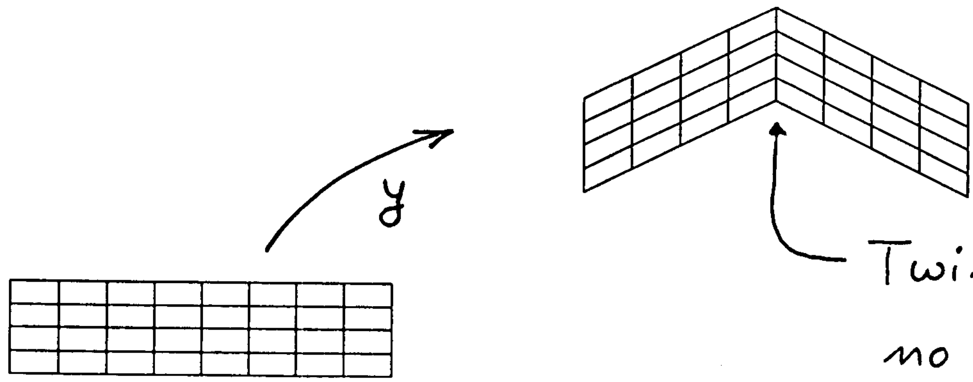
(from Olson & Hartman 1982)





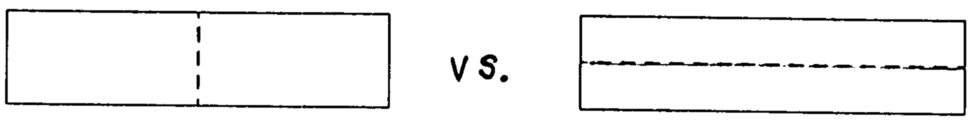


Appropriate theory?



Twin boundary
no bending!

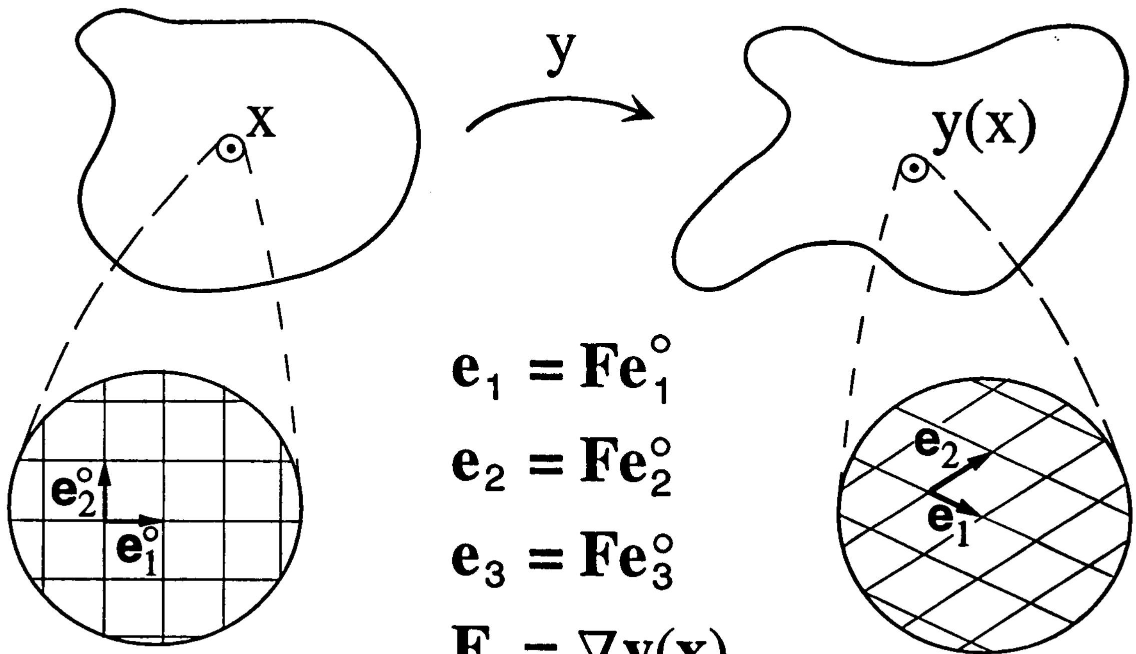
Surface energy



IDEA:

$$
\begin{tikzcd}
\boxed{\text{3d theory}} \arrow[r] \arrow[d, dashed, "?"'] & \boxed{\text{3d soln}} \arrow[d] \\
\boxed{\text{2d theory}} \arrow[r, leftrightarrow] & \boxed{\text{2d soln}}
\end{tikzcd}
$$

Continuum Theory (Single Crystal)



$$\mathbf{e}_1 = \mathbf{F}\mathbf{e}_1^\circ$$
$$\mathbf{e}_2 = \mathbf{F}\mathbf{e}_2^\circ$$
$$\mathbf{e}_3 = \mathbf{F}\mathbf{e}_3^\circ$$
$$\mathbf{F} = \nabla \mathbf{y}(\mathbf{x})$$

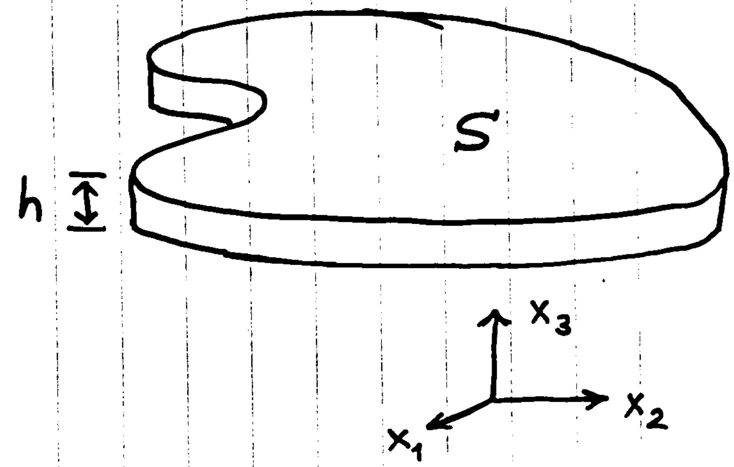
Deformation Gradient

$$F = \nabla y = \begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & \frac{\partial y_1}{\partial x_3} \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & \frac{\partial y_2}{\partial x_3} \\ \frac{\partial y_3}{\partial x_1} & \frac{\partial y_3}{\partial x_2} & \frac{\partial y_3}{\partial x_3} \end{pmatrix}$$

$$\text{Energy} = \int_\Omega W(\nabla y, T)\, dx$$

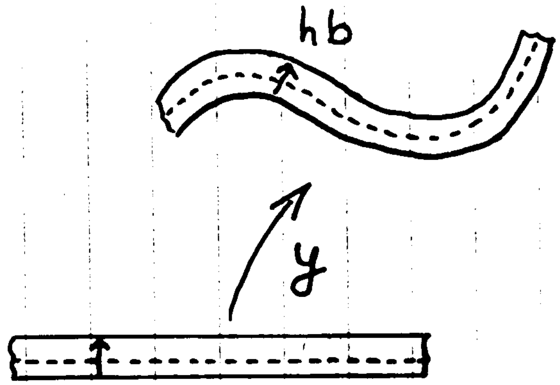
Theory of thin films

$$e^{(h)} = \int_{\Omega_h} \left\{ \varkappa^2 |\nabla^2 \tilde{y}|^2 + W(\nabla \tilde{y}) \right\} dx$$



$$h \to 0$$

$$\tilde{y}^{(h)} \longrightarrow y(x_1, x_2) + \quad x_3 \, b(x_1, x_2)$$

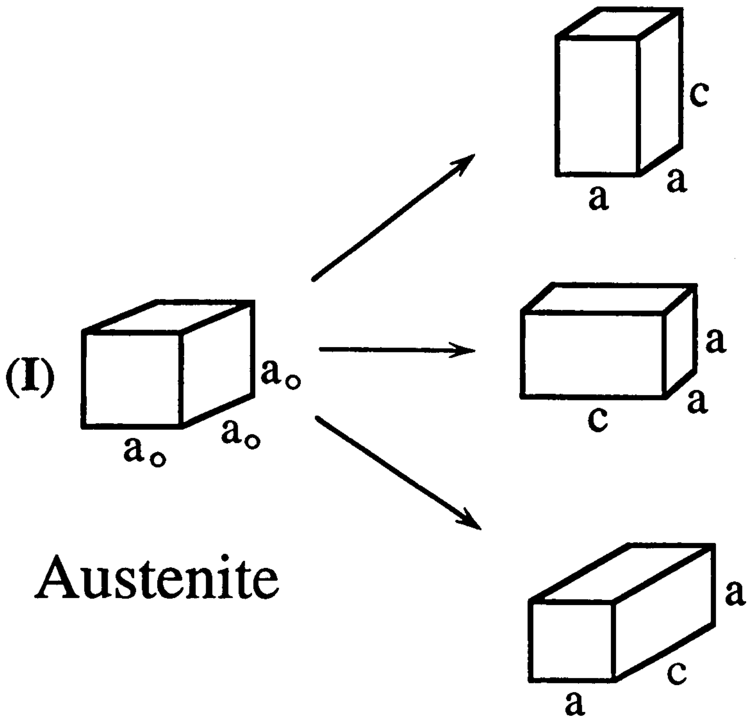


$$e^{0}[y, b] = \int_S \left\{ \varkappa^2 (\dots) + W\left(y_{,1} \,|\, y_{,2} \,|\, b \right) \right\} dx$$

$$\begin{pmatrix} \frac{\partial y_1}{\partial x_1} & \frac{\partial y_1}{\partial x_2} & b_1 \\ \frac{\partial y_2}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & b_2 \\ \frac{\partial y_3}{\partial x_1} & \frac{\partial y_2}{\partial x_2} & b_3 \end{pmatrix} \sim \left(\frac{\partial y}{\partial x_1} \,\middle|\, \frac{\partial y}{\partial x_2} \,\middle|\, b \right)$$

NO BENDING

Martensitic Phase Transformation



Austenite

Martensite

$$U_1 = \begin{pmatrix} \beta & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \alpha \end{pmatrix}$$

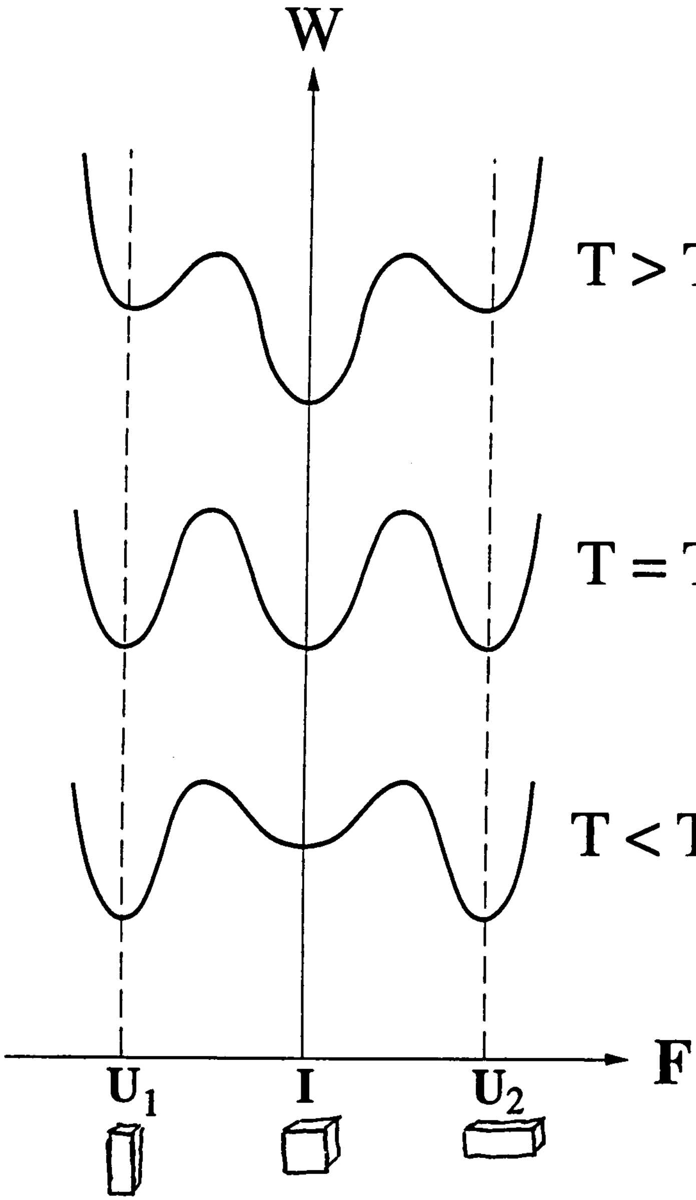
$$U_2 = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \beta & 0 \\ 0 & 0 & \alpha \end{pmatrix}$$

$$U_3 = \begin{pmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & \beta \end{pmatrix}$$

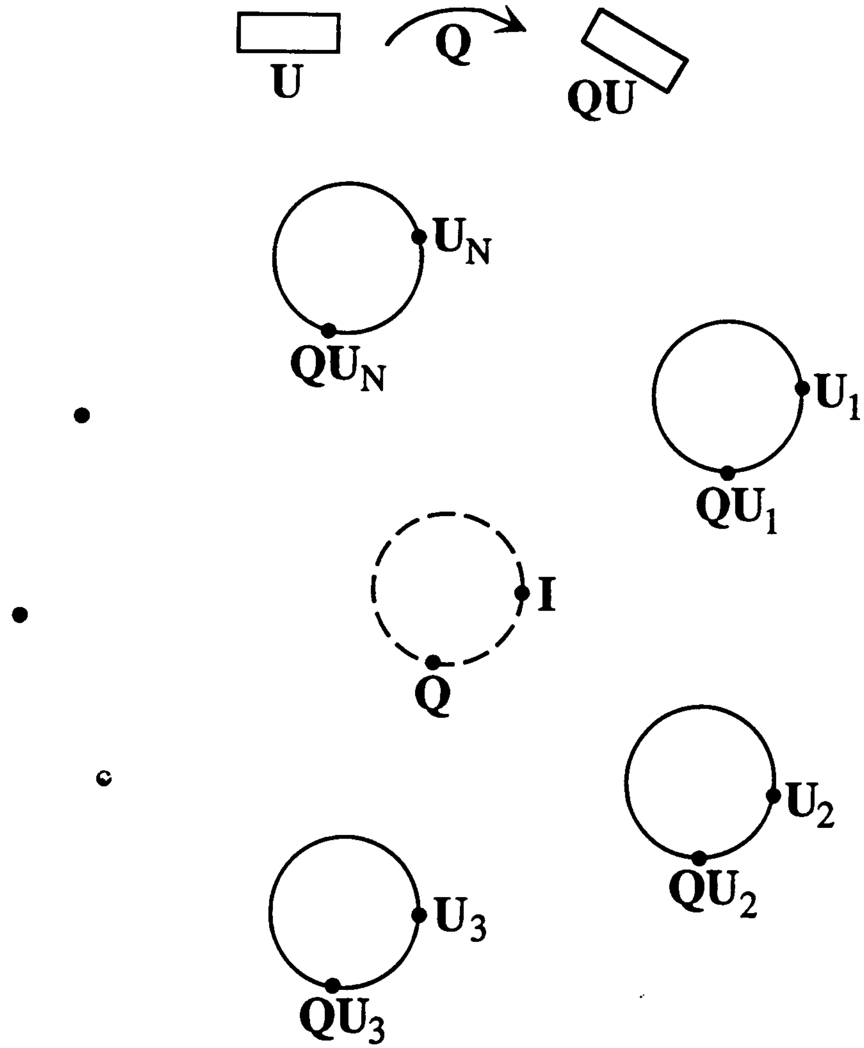
Crystallography

$\Longrightarrow$ 1. Number of Variants

2. Transformation Matrices

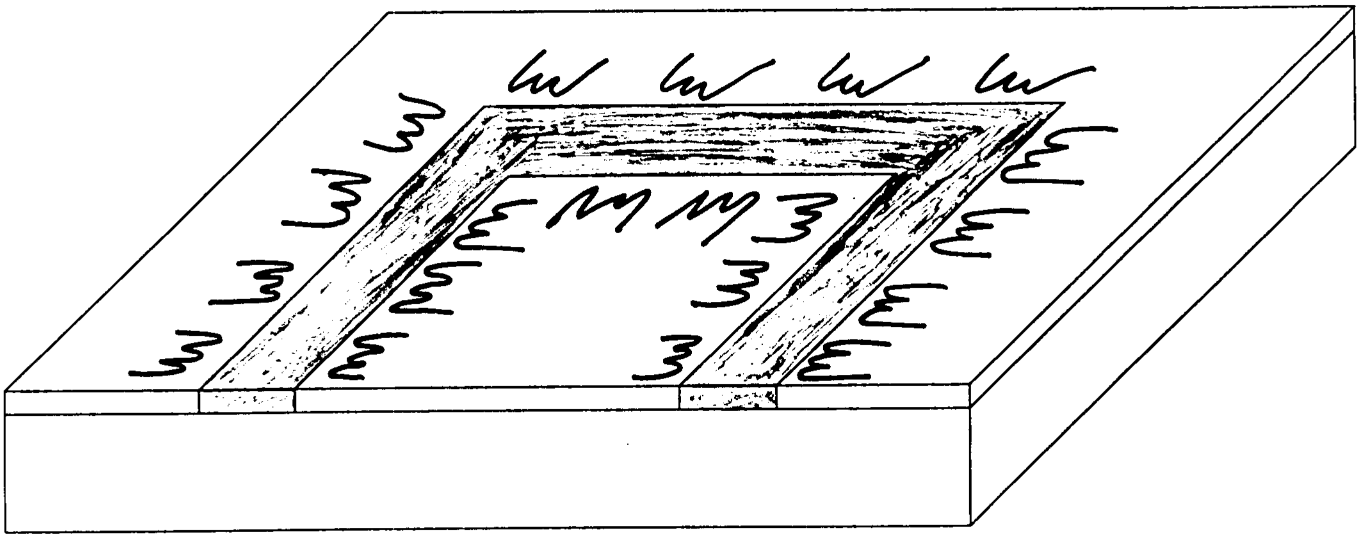


But rigid rotations do not change energy

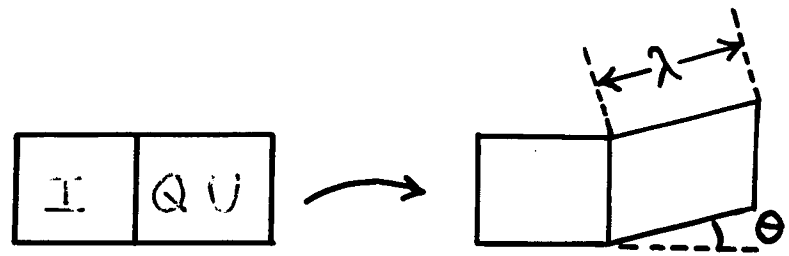


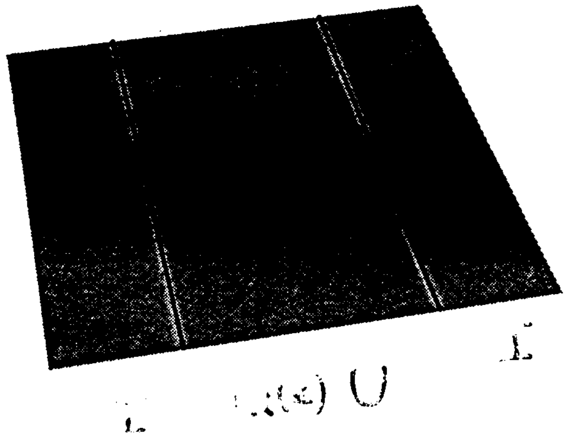
" Wells "

Possible micropump



Tunnel



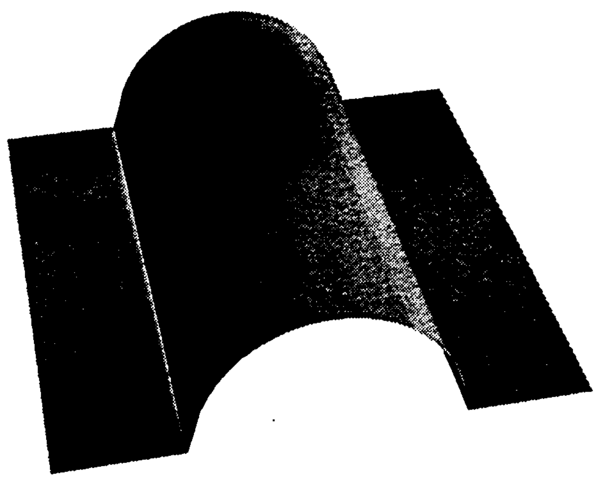


$$\theta \sim e \cdot U^2 n$$

$$\lambda = |Un|$$

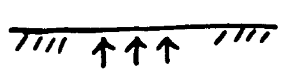
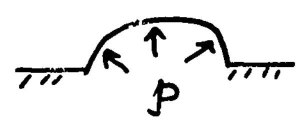
For a tunnel, $\theta = 0$, $\lambda > 1$

$$\Longleftrightarrow \begin{cases} e_3 \cdot \operatorname{adj}(U^2 - I)\, e_3 = 0 \\ \operatorname{tr} U^2 - e_3 \cdot U^2 e_3 - 2 \geqslant 0 \end{cases}$$



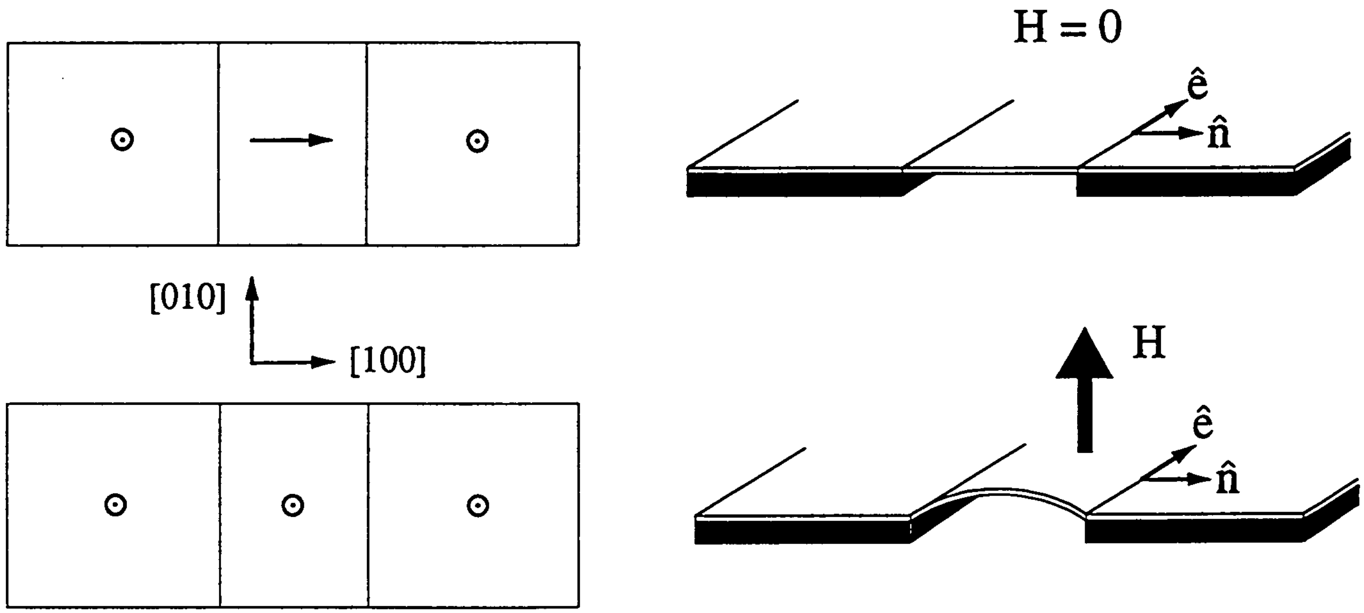
Thick substrate:

$$U = U_1 \, U^{-1}_{\text{substrate}}$$

Note: min  = 

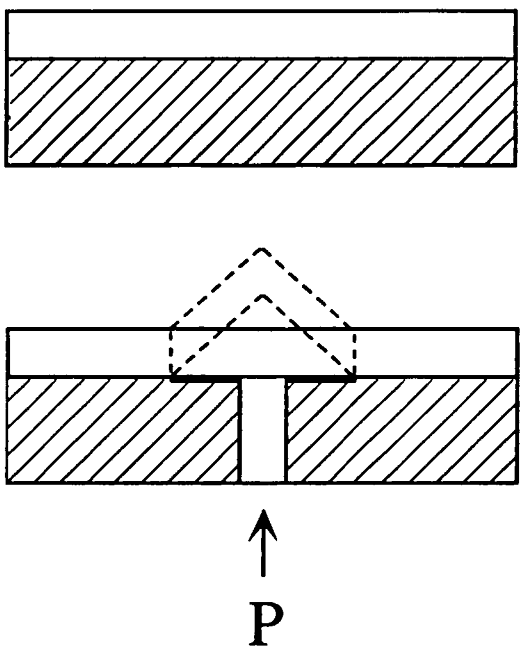
Field-induced Tunnel

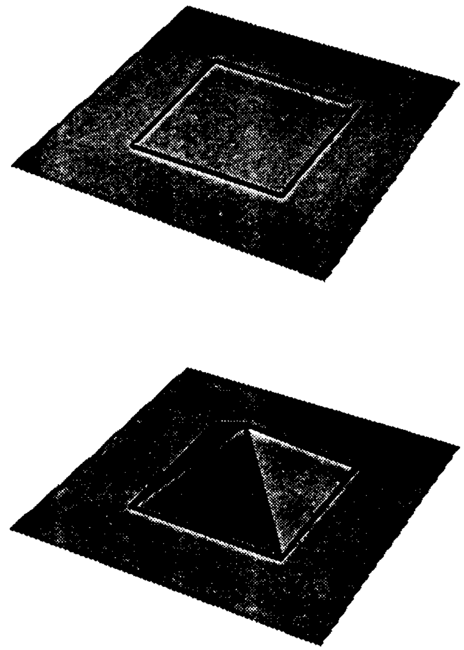
Ferro-magnetic shape-memory alloy: (001) film of Ni_2MnGa



Ferroelectric ceramic: (001) film of $PbTiO_3$

Proposed Micropump

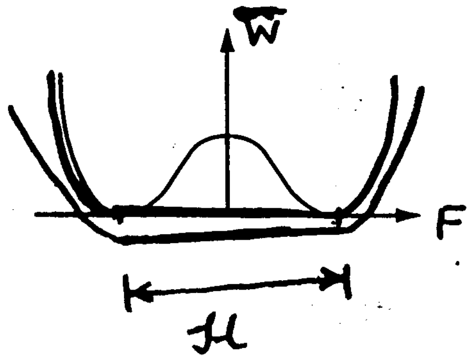




Requires

1. n - fold plane of symmetry
2. $e_3 \cdot \mathrm{cof}\ (U^2 - I)\ e_3 = 0$
3. $\mathrm{tr}\ U^2 - e_3 \cdot U^2 e_3 - 2 \geq 0$

Compute with "approximate relaxed energy"



Relaxation Theorem:

$$\min \int W = \min \int \overline{W}$$

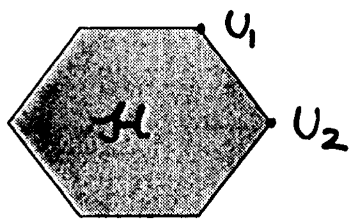
"wellposed", correct average stress, strain

BUT we do not know $\overline{W}$!

APPROXIMATE $\overline{W}$: (with Dolzmann)

Step 1: Calculate "generalized convex hulls"

$$\mathcal{H} = \{ \overline{W}(F) = 0 \}$$



Step 2: Construct $\hat{W}$ s.t.

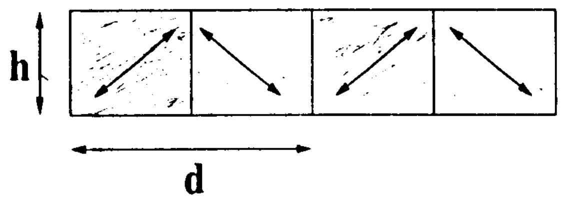
(a) $\hat{W}$ quasiconvex $\Rightarrow \min \int \hat{W}$ "wellposed"

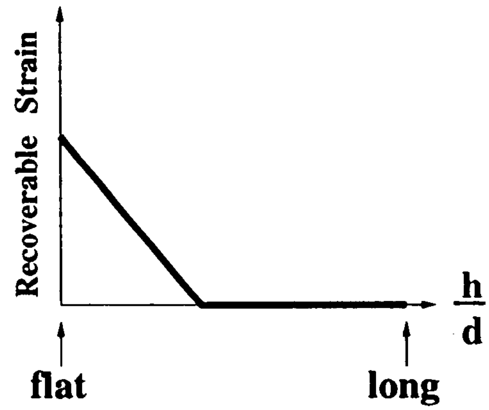
(b) $\hat{W} = 0$ on $\mathcal{H}$

(c) $\hat{W}$ grows away from $\mathcal{H}$

Recoverable Strain

- **Schematic Example :** 2-d, two well scalar problem



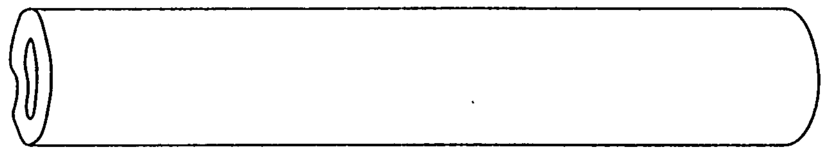


- **Application**

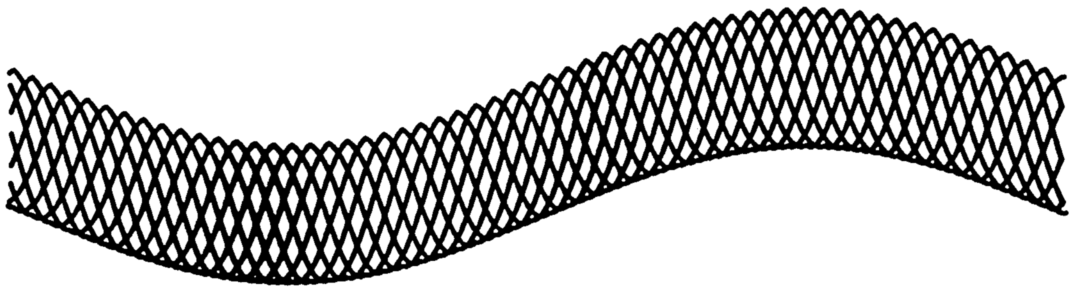
Texture	Recoverable Strains (%)			
	Ti-Ni		Cu-Zn-Al	
	long	flat	long	flat
random	2.3	2.3	1.7	1.7
{110} sputtered	2.3	2.3	1.7	1.7
{111} film	5.3	8.1	1.9	5.9
{100} film	2.3	2.3	7.1	7.1

Current activities

Flagella: Strings, rods and tubes



"two director
Cosserat string"



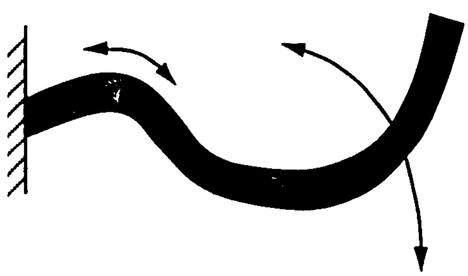
Effective continuum theory — with R.D. James

Atomistic-continuum linkage — with K.M. Rabe, R.D. James, G. Friesecke

Property ⇔ Continuum ⇔Phase transformation ⇔ Atomistic

Use "change of scale" methods to propose computational strategies for atomistics

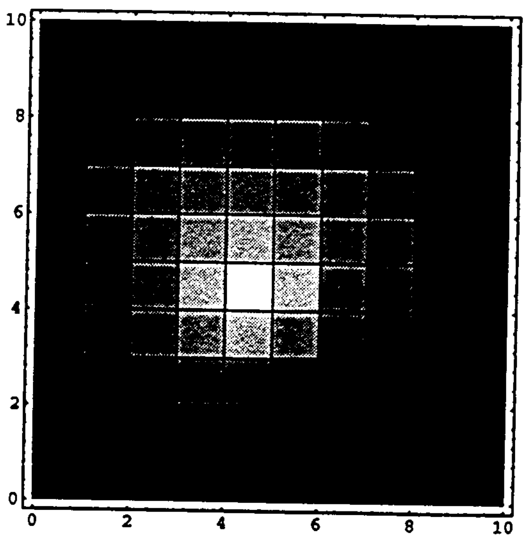
Dynamics — P. Purohit



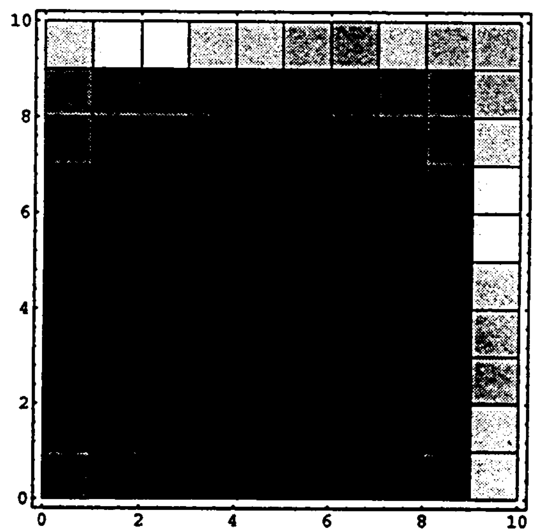
Random walker with a purpose

"get away from the light"

1. Sit quiet for some time and then take a step in a random direction
2. Frequency of steps proportional to intensity.



Intensity



Position